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High-Order Compact ADI Methods for Parabolic Equations

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Dedicated to Professor Michael Navon on the occasion of his 65th birthday.

Abstract—In this paper we develop a sixth-order compact scheme coupled with Alternating Direction Implicit (ADI) methods and apply it to parabolic equations in both 2-D and 3-D. Unconditional stability is proved for linear diffusion problems with periodic boundary conditions. Numerical examples supporting our theoretical analysis are provided.

Keywords—High-order compact schemes, Parabolic equations, ADI method.

1. INTRODUCTION

Recently, due to their high accuracy, compactness (therefore, consuming less memory space), and better resolution for high frequency waves [1], the high-order compact (HOC) difference methods have seen increasing popularity in computational acoustics [2–4], computational electromagnetics [5,6], oceanic applications [7–9], and many other applications [10,11], where very accurate simulations can be carried out over very long time periods and far distances. To date, most investigations are focused on hyperbolic equations (e.g., [12–14] and references cited therein), though there are some published work [12,15–20] on solving parabolic equations using HOC. However, the second derivative terms received much less attention [20, p. 503], especially the theoretical analysis for problems in high-dimensional spaces.

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In [21,22], we applied HOC difference methods to some one-dimensional time-dependent problems containing high-order derivatives. Here we extend our previous application to high-dimensional parabolic equations. Notice that most work on compact ADI methods [15,17–19] are restricted to fourth-order, and their formulations of HOC are quite different and seem more complicated than ours. In this paper we develop the sixth-order compact scheme using Alternating Direction Implicit (ADI) methods and apply it to parabolic equations in both 2-D and 3-D. Unconditional stability is proved for linear diffusion problem with periodic boundary conditions. Numerical examples supporting our theoretical analysis are provided.

The contents of this paper are as follows. In Section 2, we describe the detailed numerical algorithms and prove the unconditional stability for 2-D problems with periodic boundary conditions. Stability analysis is extended to 3-D periodic problems in Section 3. In Section 4, we present four numerical examples: two linear diffusion problems, the Burgers' equation, and a system of nonlinear parabolic equations. Our numerical results show that high accuracy can be obtained very efficiently by the high-order compact schemes. We conclude the paper in Section 5.

2. NUMERICAL ALGORITHMS

2.1. Spatial Discretization

A finite-difference approach is employed to discretize the space dimension. Spatial derivatives are evaluated by the compact finite difference scheme [1]. Given any scalar pointwise value f, the derivatives of f are obtained by solving a tridiagonal or pentadiagonal system. Much work has been done in deriving such formulas and showing that the compact scheme has smaller dispersive error compared to the same order explicit difference scheme [1,21].

For simplicity, we consider a uniform 1-D mesh, consisting of N points: $1,2,\dots,i-1,i,$ $i+1,\dots,N$. We denote the mesh size $h = x_{i+1} - x_i$.

For the first derivatives at interior nodes, we have the formula [1]

$$\alpha f'_{i-1} + f'_i + \alpha f'_{i+1} = b\frac{f_{i+2} - f_{i-2}}{4h} + a\frac{f_{i+1} - f_{i-1}}{2h}, \tag{1}$$

which provides an α-family of fourth-order tridiagonal schemes with

$$a = \frac{2}{3}(\alpha + 2), \qquad b = \frac{1}{3}(4\alpha - 1).$$

Its truncation error is $(4/5!)(3\alpha - 1)h^4 f^{(5)}$ [1, p. 18]. When $\alpha = 1/3$, the scheme becomes sixth-order accurate, in which case $a = 14/9$, $b = 1/9$.

For the second derivatives at interior nodes, we have the formula [1]

$$\alpha f''_{i-1} + f''_i + \alpha f''_{i+1} = b\frac{f_{i+2} - 2f_i + f_{i-2}}{4h^2} + a\frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}, \tag{2}$$

which provides an α-family of fourth-order tridiagonal schemes with

$$a = \frac{4}{3}(1 - \alpha), \qquad b = \frac{1}{3}(-1 + 10\alpha).$$

Its truncation error is $(-4/6!)(11\alpha - 2)h^4 f^{(6)}$ [1 p. 19]. When $\alpha = 2/11$, the scheme becomes sixth-order accurate, in which case $a = 12/11$, $b = 3/11$.

For those near boundary nodes, approximation formulas for the derivatives of non-periodic problems can be derived by one-sided schemes. First we list some formulas for the first derivatives derived in [23].

At boundary point 1, the sixth-order formula is [23]

$$f_1' + \alpha f_2' = (c_1 f_1 + c_2 f_2 + c_3 f_3 + c_4 f_4 + c_5 f_5 + c_6 f_6 + c_7 f_7)/h,$$

where

$$\alpha = 5, \qquad c_1 = \frac{-197}{60}, \qquad c_2 = \frac{-5}{12}, \qquad c_3 = 5,$$

$$c_4 = \frac{-5}{3}, \qquad c_5 = \frac{5}{12}, \qquad c_6 = \frac{-1}{20}, \qquad c_7 = 0.$$

At boundary point 2, the sixth-order formula is [23]

$$\alpha f_1' + f_2' + \alpha f_3' = (c_1 f_1 + c_2 f_2 + c_3 f_3 + c_4 f_4 + c_5 f_5 + c_6 f_6 + c_7 f_7)/h,$$

where

$$\alpha = \frac{2}{11}, \qquad c_1 = \frac{-20}{33}, \qquad c_2 = \frac{-35}{132}, \qquad c_3 = \frac{34}{33},$$

$$c_4 = \frac{-7}{33}, \qquad c_5 = \frac{2}{33}, \qquad c_6 = \frac{-1}{132}, \qquad c_7 = 0.$$

At boundary point $N-1$, the sixth-order formula is [23]

$$\alpha f_{N-2}' + f_{N-1}' + \alpha f_N' = (c_1 f_N + c_2 f_{N-1} + c_3 f_{N-2} + c_4 f_{N-3} + c_5 f_{N-4} + c_6 f_{N-5} + c_7 f_{N-6})/h,$$

where $\alpha = 2/11$. The rest coefficients are the opposite of those given for point 2 (i.e., the signs are reversed).

At boundary point N, the sixth-order formula is [23]

$$\alpha f_{N-1}' + f_N' = (c_1 f_N + c_2 f_{N-1} + c_3 f_{N-2} + c_4 f_{N-3} + c_5 f_{N-4} + c_6 f_{N-5} + c_7 f_{N-6})/h,$$

where $\alpha = 5$. The rest coefficients are the opposite of those given for point 1 (i.e., the signs are reversed).

In [1], Lele only presented the formulation of the third-order compact scheme for approximating the second derivatives at those near boundary points. Below we derive the sixth-order compact formulas at those near boundary points.

At boundary point 1, we construct the sixth-order formula

$$f_1'' + \alpha f_2'' = (c_1 f_1 + c_2 f_2 + c_3 f_3 + c_4 f_4 + c_5 f_5 + c_6 f_6 + c_7 f_7)/h^2,$$

where the coefficients can be found by matching the Taylor series expansions up to order of h^7, which gives us the following linear system

$$c_1 + c_2 + c_3 + c_4 + c_5 + c_6 + c_7 = 0,$$

$$c_2 + 2c_3 + 3c_4 + 4c_5 + 5c_6 + 6c_7 = 0,$$

$$c_2 + 2^2 c_3 + 3^2 c_4 + 4^2 c_5 + 5^2 c_6 + 6^2 c_7 = (2!)(1+\alpha),$$

$$c_2 + 2^3 c_3 + 3^3 c_4 + 4^3 c_5 + 5^3 c_6 + 6^3 c_7 = (3!)\alpha,$$

$$c_2 + 2^4 c_3 + 3^4 c_4 + 4^4 c_5 + 5^4 c_6 + 6^4 c_7 = \frac{4!}{2!}\alpha,$$

$$c_2 + 2^5 c_3 + 3^5 c_4 + 4^5 c_5 + 5^5 c_6 + 6^5 c_7 = \frac{5!}{3!}\alpha,$$

$$c_2 + 2^6 c_3 + 3^6 c_4 + 4^6 c_5 + 5^6 c_6 + 6^6 c_7 = \frac{6!}{4!}\alpha,$$

$$c_2 + 2^7 c_3 + 3^7 c_4 + 4^7 c_5 + 5^7 c_6 + 6^7 c_7 = \frac{7!}{5!}\alpha.$$

The solution to the above system is

$$c_1 = 2077/157, \qquad c_2 = -2943/110, \qquad c_3 = 573/44, \qquad c_4 = 167/99, \tag{3}$$

$$c_5 = -18/11, \qquad c_6 = 57/110, \qquad c_7 = -131/1980, \qquad \alpha = 126/11. \tag{4}$$

At boundary point 2, we can construct the sixth-order formula

$$\alpha f_1'' + f_2'' + \alpha f_3'' = \left(c_1 f_1 + c_2 f_2 + c_3 f_3 + c_4 f_4 + c_5 f_5 + c_6 f_6 + c_7 f_7\right)/h^2.$$

Matching the Taylor series expansions up to order of h^7 gives us the following linear system

$$c_1 + c_2 + c_3 + c_4 + c_5 + c_6 + c_7 = 0,$$

$$c_2 + 2c_3 + 3c_4 + 4c_5 + 5c_6 + 6c_7 = 0,$$

$$c_2 + 2^2 c_3 + 3^2 c_4 + 4^2 c_5 + 5^2 c_6 + 6^2 c_7 = (2!)(1 + 2\alpha),$$

$$c_2 + 2^3 c_3 + 3^3 c_4 + 4^3 c_5 + 5^3 c_6 + 6^3 c_7 = (3!)(1 + 2\alpha),$$

$$c_2 + 2^4 c_3 + 3^4 c_4 + 4^4 c_5 + 5^4 c_6 + 6^4 c_7 = \frac{4!}{2!}(1 + 2^2\alpha),$$

$$c_2 + 2^5 c_3 + 3^5 c_4 + 4^5 c_5 + 5^5 c_6 + 6^5 c_7 = \frac{5!}{3!}(1 + 2^3\alpha),$$

$$c_2 + 2^6 c_3 + 3^6 c_4 + 4^6 c_5 + 5^6 c_6 + 6^6 c_7 = \frac{6!}{4!}(1 + 2^4\alpha),$$

$$c_2 + 2^7 c_3 + 3^7 c_4 + 4^7 c_5 + 5^7 c_6 + 6^7 c_7 = \frac{7!}{5!}(1 + 2^5\alpha),$$

which has the solution

$$c_1 = 585/512, \qquad c_2 = -141/64, \qquad c_3 = 459/512, \qquad c_4 = 9/32, \tag{5}$$

$$c_5 = -81/512, \qquad c_6 = 3/64, \qquad c_7 = -3/512, \qquad \alpha = 11/128. \tag{6}$$

Similarly, at boundary point $N-1$, the sixth-order formula is

$$\alpha f_{N-2}'' + f_{N-1}'' + \alpha f_N'' = \left(c_1 f_N + c_2 f_{N-1} + c_3 f_{N-2} + c_4 f_{N-3} + c_5 f_{N-4} + c_6 f_{N-5} + c_7 f_{N-6}\right)/h^2,$$

where the coefficients are given by (5),(6). And at boundary point N, the sixth-order formula is

$$\alpha f_{N-1}'' + f_N'' = \left(c_1 f_N + c_2 f_{N-1} + c_3 f_{N-2} + c_4 f_{N-3} + c_5 f_{N-4} + c_6 f_{N-5} + c_7 f_{N-6}\right)/h^2,$$

where the coefficients are given by (3),(4).

2.2. Temporal Discretization

Considering the efficiency of Alternating Direction Implicit (ADI) methods for solving 2-D or 3-D problems, we will use the ADI method in our implementation. Though ADI coupled with fourth-order compact schemes have been investigated in [15,17–19], our derivations are quite different and much simpler as shown below. For clarity and generality, we present the algorithm for the following 2-D parabolic equation:

$$u_t = \nu(u_{xx} + u_{yy}) + F(x, y, t), \qquad (x, y, t) \in \Omega \times (0, T], \tag{7}$$

$$u(x, y, 0) = G(x, y), \qquad (x, y) \in \Omega, \tag{8}$$

$$u(x, y, t)|_{\partial\Omega} = H(x, y), \qquad t \in [0, T], \tag{9}$$

where the diffusion coefficient ν is a positive constant, $\Omega \equiv [0, 1]^2$, and $\partial\Omega$ is the boundary of the domain.

To develop our high-order compact scheme, Ω is divided into a uniform mesh in each direction, i.e.,

$$x_i = (i - 1)\Delta x, \quad i = 1, \ldots, N_x; \qquad y_j = (j - 1)\Delta y, \quad j = 1, \ldots, N_y,$$

where $\Delta x, \Delta y$ are the mesh sizes in the x- and y-direction, respectively. We denote u_{ij}^n the approximate solution of $u(i\Delta x, j\Delta y, n\Delta t)$, where Δt is the time step.

By applying the Peaceman-Rachford ADI method [24] to (7), we have

$$\frac{u_{ij}^{n+1/2} - u_{ij}^n}{0.5\Delta t} = \nu \left[(u_{xx})_{ij}^{n+1/2} + (u_{yy})_{ij}^n \right] + (F)_{ij}^{n+1/2}, \tag{10}$$

$$\frac{u_{ij}^{n+1} - u_{ij}^{n+1/2}}{0.5\Delta t} = \nu \left[(u_{xx})_{ij}^{n+1/2} + (u_{yy})_{ij}^{n+1} \right] + (F)_{ij}^{n+1/2}, \tag{11}$$

where $(F)_{ij}^{n+1/2} = F(x_i, y_j, (n + 1/2)\Delta t)$. Then all the derivatives in (10),(11) are approximated by the sixth-order compact formulas developed in Section 2.1. For example, we can write

$$(u_{xx})_{,j} = \frac{1}{(\Delta x)^2} A^{-1} B u_{,j}, \tag{12}$$

where A and B are the corresponding $N_x \times N_x$ triangular and sparse matrices, $u_{,j} = (u_{1,j}, u_{2,j}, \ldots, u_{N_x,j})'$ is the solution vector at the j^{th} row. Substituting (12) into (10) gives us

$$\left(I_x - \frac{1}{2}\nu \frac{\Delta t}{(\Delta x)^2} A^{-1} B \right) u_{,j}^{n+1/2} = u_{,j}^n + \frac{1}{2}\Delta t \left[\nu \left(u_{yy} \right)_{,j}^n + F_{,j}^{n+1/2} \right], \tag{13}$$

where I_x denotes the $N_x \times N_x$ identity matrix.

Similarly for the equation (11) in the y-direction, we can obtain

$$\left(I_y - \frac{1}{2}\nu \frac{\Delta t}{(\Delta y)^2} C^{-1} D \right) u_{i,}^{n+1} = u_{i,}^{n+1/2} + \frac{1}{2}\Delta t \left[\nu \left(u_{xx} \right)_{i,}^{n+1/2} + F_{i,}^{n+1/2} \right], \tag{14}$$

by using

$$(u_{yy})_{i,} = \frac{1}{(\Delta y)^2} C^{-1} D u_{i,}$$

where C and D are the corresponding $N_y \times N_y$ triangular and sparse matrices, $u_{i,} = (u_{i,1}, u_{i,2}, \ldots, u_{i,N_y})'$ is the solution vector at the i^{th} column, and I_y denotes the $N_y \times N_y$ identity matrix.

We like to mention that the above scheme has truncation error $O((\Delta t)^2, (\Delta x)^6, (\Delta y)^6)$. Note that the coefficient matrices of (13) and (14) are time-independent, hence, we can store the inverse of those coefficient matrices before the time- marching in the implementation for computational efficiency.

2.3. Stability Analysis

To study the stability of our scheme, we use the von Neumann stability analysis. For simplicity, we assume $F \equiv 0$ in (10),(11), and u is periodic in both x and y.

For the sixth-order compact scheme (2) for a periodic problem, the matrices A and B have the property

$$Au_i = \alpha u_{i-1} + u_i + \alpha u_{i+1}, \qquad Bu_i = \frac{b}{4}(u_{i+2} - 2u_i + u_{i-2}) + a(u_{i+1} - 2u_i + u_{i-1}).$$

Let

$$u_{ij}^n = \xi^n e^{I(w_x i + w_y j)}, \qquad I = \sqrt{-1}$$

be the solution of (10),(11), where $w_x = 2\pi\Delta x/l_x$ and $w_y = 2\pi\Delta y/l_y$ are phase angles with wavelengths l_x and l_y, respectively. It is easy to verify that

$$Ae^{Iw_x i} = e^{Iw_x i}\left(\alpha e^{Iw_x} + 1 + \alpha e^{-Iw_x}\right) = e^{Iw_x i}\left(2\alpha\cos w_x + 1\right),$$

$$Be^{Iw_x i} = e^{Iw_x i}\left[\frac{b}{4}\left(e^{I2w_x} - 2 + e^{-I2w_x}\right) + a\left(e^{Iw_x} - 2 + e^{-Iw_x}\right)\right] = e^{Iw_x i}\left[-b\sin^2 w_x - 4a\sin^2\frac{w_x}{2})\right].$$

Therefore, we have

$$\begin{aligned}(u_{xx})_{ij}^{n+1/2} &= \frac{1}{(\Delta x)^2}A^{-1}Bu_{ij}^{n+1/2} \\ &= \frac{u_{ij}^{n+1/2}}{(\Delta x)^2}\frac{(-b\sin^2 w_x - 4a\sin^2(w_x/2))}{(2\alpha\cos w_x + 1)}.\end{aligned} \tag{15}$$

We denote

$$m_x = \frac{1}{2}\frac{\nu\Delta t}{(\Delta x)^2}, \qquad m_y = \frac{1}{2}\frac{\nu\Delta t}{(\Delta y)^2},$$

and

$$\gamma_x = \frac{(-b\sin^2 w_x - 4a\sin^2(w_x/2))}{(2\alpha\cos w_x + 1)}, \qquad \gamma_y = \frac{(-b\sin^2 w_y - 4a\sin^2(w_y/2))}{(2\alpha\cos w_y + 1)}.$$

Hence, (15) can be written as

$$(u_{xx})_{ij}^{n+1/2} = \frac{1}{(\Delta x)^2}A^{-1}Bu_{ij}^{n+1/2} = \frac{1}{(\Delta x)^2}\gamma_x u_{ij}^{n+1/2}. \tag{16}$$

Similarly, it is easy to find that

$$(u_{yy})_{ij}^{n+1} = \frac{1}{(\Delta y)^2}C^{-1}Du_{ij}^{n+1} = \frac{1}{(\Delta y)^2}\gamma_y u_{ij}^{n+1}. \tag{17}$$

Substituting (15) and (16) into (10) with $F = 0$, we obtain

$$(1 - m_x\gamma_x)\, u_{ij}^{n+1/2} = (1 + m_y\gamma_y)\, u_{ij}^n. \tag{18}$$

In the same way, from (11) we can easily obtain

$$(1 - m_y\gamma_y)\, u_{ij}^{n+1} = (1 + m_x\gamma_x)\, u_{ij}^{n+1/2}. \tag{19}$$

From (18),(19), we see that the amplification factor

$$|\xi| = \left|\frac{u_{ij}^{n+1}}{u_{ij}^{n+1/2}}\right| \cdot \left|\frac{u_{ij}^{n+1/2}}{u_{ij}^n}\right| = \left|\frac{1 + m_x\gamma_x}{1 - m_y\gamma_y} \cdot \frac{1 + m_y\gamma_y}{1 - m_x\gamma_x}\right| \le 1,$$

whenever $\gamma_x \le 0$ and $\gamma_y \le 0$ hold true. It is easy to see that for our special sixth-order scheme (2) with

$$\alpha = \frac{2}{11}, \qquad a = \frac{12}{11}, \qquad b = \frac{3}{11}, \tag{20}$$

$\gamma_x \le 0$ and $\gamma_y \le 0$ hold true, which means that our scheme (10),(11) is unconditionally stable in this case.

3. EXTENSIONS TO 3-D COMPACT ADI SCHEMES

The above compact ADI scheme can be extended directly to 3-D case, such as

$$u_t = \nu\left(u_{xx} + u_{yy} + u_{zz}\right) + F(x,y,z,t), \qquad (x,y,z,t) \in \Omega \times (0,T]. \tag{21}$$

By applying the Douglas ADI method [25] to (21), we have

$$\frac{u_{ijk}^{n+1/3} - u_{ijk}^{n}}{\Delta t} = \nu\left[\frac{1}{2}\left((u_{xx})_{ijk}^{n+1/3} + (u_{xx})_{ijk}^{n}\right) + (u_{yy})_{ijk}^{n} + (u_{zz})_{ijk}^{n}\right] + (F)_{ijk}^{n+1/2}, \tag{22}$$

$$\frac{u_{ijk}^{n+2/3} - u_{ijk}^{n+1/3}}{0.5\Delta t} = \nu\left[(u_{yy})_{ijk}^{n+2/3} - (u_{yy})_{ijk}^{n}\right], \tag{23}$$

$$\frac{u_{ijk}^{n+1} - u_{ijk}^{n+2/3}}{0.5\Delta t} = \nu\left[(u_{zz})_{ijk}^{n+1} - (u_{zz})_{ijk}^{n}\right], \tag{24}$$

where $(F)_{ijk}^{n+1/2} = F(x_i, y_j, z_k, (n+1/2)\Delta t)$, and u_{ijk}^n denotes the approximate solution of $u(x_i, y_j, z_k, t_n)$. Then all the derivatives in (22)–(24) are approximated by the sixth-order compact formulas developed in Section 2.1.

Applying the similar technique used for 2-D in Section 2.3, we can prove unconditional stability of our scheme (22)–(24) with periodic boundary conditions. For stability analysis, we assume $F = 0$. In 3-D case, we let

$$u_{ijk}^n = \xi^n e^{I(w_x i + w_y j + w_z k)}, \qquad I = \sqrt{-1},$$

be the solution of (22)–(24).

Similar to the 2-D case, we can easily obtain

$$(u_{xx})_{ijk}^n = \frac{1}{(\Delta x)^2}\gamma_x u_{ijk}^n, (u_{yy})_{ijk}^n = \frac{1}{(\Delta y)^2}\gamma_y u_{ijk}^n, (u_{zz})_{ijk}^n = \frac{1}{(\Delta z)^2}\gamma_z u_{ijk}^n. \tag{25}$$

Substituting (25) into (22)-(24), we have

$$\left(1 - m_x\gamma_x\right) u_{ijk}^{n+1/3} = u_{ijk}^n + m_x\gamma_x u_{ijk}^n + 2m_y\gamma_y u_{ijk}^n + 2m_z\gamma_z u_{ijk}^n, \tag{26}$$

$$\left(1 - m_y\gamma_y\right) u_{ijk}^{n+2/3} = u_{ijk}^{n+1/3} - m_y\gamma_y u_{ijk}^n, \tag{27}$$

$$\left(1 - m_z\gamma_z\right) u_{ijk}^{n+1} = u_{ijk}^{n+2/3} - m_z\gamma_z u_{ijk}^n. \tag{28}$$

Multiplying (28) by $(1 - m_y\gamma_y)$ and combining the resultant with (27), we obtain

$$\left(1 - m_y\gamma_y\right)\left(1 - m_z\gamma_z\right) u_{ijk}^{n+1} = u_{ijk}^{n+1/3} - m_y\gamma_y u_{ijk}^n - m_z\gamma_z\left(1 - m_y\gamma_y\right) u_{ijk}^n. \tag{29}$$

Multiplying (29) by $(1 - m_x\gamma_x)$ and combining the resultant with (26), we obtain

$$\left(1 - m_x\gamma_x\right)\left(1 - m_y\gamma_y\right)\left(1 - m_z\gamma_z\right) u_{ijk}^{n+1} = \left(1 + m_x\gamma_x + 2m_y\gamma_y + 2m_z\gamma_z\right) u_{ijk}^n$$

$$-m_y\gamma_y\left(1 - m_x\gamma_x\right) u_{ijk}^n - m_z\gamma_z\left(1 - m_x\gamma_x\right)\left(1 - m_y\gamma_y\right) u_{ijk}^n$$

$$= \left(1 + m_x\gamma_x + m_y\gamma_y + m_z\gamma_z + m_x\gamma_x m_y\gamma_y + m_z\gamma_z m_x\gamma_x + m_z\gamma_z m_y\gamma_y - m_x\gamma_x m_y\gamma_y m_z\gamma_z\right) u_{ijk}^n,$$

which gives us the amplification factor

$$|\xi| = \left|\frac{u_{ijk}^{n+1}}{u_{ijk}^{n}}\right| = \left|\frac{(1 + m_x\gamma_x + m_y\gamma_y + m_z\gamma_z + m_x\gamma_x m_y\gamma_y + m_z\gamma_z m_x\gamma_x + m_z\gamma_z m_y\gamma_y - m_x\gamma_x m_y\gamma_y m_z\gamma_z)}{(1 - m_x\gamma_x)(1 - m_y\gamma_y)(1 - m_z\gamma_z)}\right|$$

$$= \left|\frac{(1 + m_x\gamma_x + m_y\gamma_y + m_z\gamma_z + m_x\gamma_x m_y\gamma_y + m_z\gamma_z m_x\gamma_x + m_z\gamma_z m_y\gamma_y - m_x\gamma_x m_y\gamma_y m_z\gamma_z)}{(1 - m_x\gamma_x - m_y\gamma_y - m_z\gamma_z + m_x\gamma_x m_y\gamma_y + m_z\gamma_z m_x\gamma_x + m_z\gamma_z m_y\gamma_y - m_x\gamma_x m_y\gamma_y m_z\gamma_z)}\right|. \tag{30}$$

From Section 2.3, we know that our special sixth-order scheme (2) with

$$\alpha = \frac{2}{11}, \qquad a = \frac{12}{11}, \qquad b = \frac{3}{11}, \tag{31}$$

gurantees $\gamma_x \le 0$ and $\gamma_y \le 0$ for all modes, which fact along with (30) shows that $|\xi| \le 1$, i.e., our scheme (22)–(24) is proved to be unconditionally stable.

REMARK. Similar analysis can be carried out for other ADI schemes (e.g., [26]), which references can be found in books such as [27,28]. The stability for nonperiodic cases can be pursued using other methods such as [14,20], which is much more complicated and shall be further studied.

4. NUMERICAL EXAMPLES

In this section, four numerical examples are carried out. The first two are linear diffusion problems with periodic boundary conditions, which are used to confirm our theoretical analysis. Then we generalize the ADI scheme to the Burgers' equation, and a system of nonlinear reaction-diffusion equations. Though robust theoretical analysis for nonlinear problems is unavailable presently, the numerical results show that such ADI methods can be easily extended to more complicated problems. For simplicity, we fix our problem domain $\Omega = (0,1) \times (0,1)$ in all examples. All computations are performed under MATLAB 6.0 installed on a laptop with Intel Pentium 3 processor at 533 MHz and 224 MB RAM.

EXAMPLE 1. Consider the linear diffusion problem

$$u_t = \frac{1}{32\pi^2}(u_{xx} + u_{yy}), \qquad (x,y) \in \Omega, \quad 0 < t < 1 \tag{32}$$

with periodic boundary conditions in both x and y directions and properly selected initial condition so that the exact solution is given by

$$u(x,y,t) = e^{-t}\sin(4\pi x)\sin(4\pi y). \tag{33}$$

We solved this problem by the ADI method (10),(11) using the sixth-order scheme (2) to approximate those derivatives. To confirm the theoretical accuracy $O((\Delta t)^2, (\Delta x)^6, (\Delta y)^6)$, we first solved the problem with a fixed mesh size $\Delta x = \Delta y = 1/50$, and various time step sizes. The results are presented in Table 1, which shows the convergence rate of $O((\Delta t)^2)$ very well. To investigate the convergence rate in space, we then solved the problem with a fixed time step size $\Delta t = 1/1000$, and various mesh sizes. The results are presented in Table 2, which shows the convergence rate of $O((\Delta x)^6)$ very well. Furthermore, the CPU time agrees well with our implementation too, since we use the LU solver, whose computational cost is $O(N^2)$, where N is the number of unknowns.

Table 1. Maximum error for Example 1 at $t = 1$ with fixed mesh size $\Delta x = \Delta y = 1/50$.

Time step size	Maximum error	Convergence rate in term of Δt	CPU time in seconds
$\Delta t = 1/10$	7.6332e − 5		5.50 s
$\Delta t = 1/20$	1.9058e − 5	2.0019	8.96 s
$\Delta t = 1/40$	4.7431e − 6	2.0065	15.93 s
$\Delta t = 1/80$	1.0893e − 6	2.0260	30.04 s
$\Delta t = 1/160$	2.7000e − 7	2.1088	61.02 s

Table 2. Maximum error for Example 1 at $t = 1$ with fixed time step size $\Delta t = 1/1000$.

Mesh size	Maximum error	Convergence rate in term of Δx	CPU time in seconds
$\Delta x = \Delta y = 1/10$	4.3608e − 4		27.12 s
$\Delta x = \Delta y = 1/20$	6.3710e − 6	6.0969	97.22 s
$\Delta x = \Delta y = 1/40$	1.0058e − 7	5.9851	332.19 s
$\Delta x = \Delta y = 1/80$	1.6257e − 9	5.9511	1331.30 s

EXAMPLE 2. Now we consider another diffusion problem

$$u_t = u_{xx} + u_{yy} + f(x, y, t), \qquad (x, y) \in \Omega, \quad 0 < t < 1 \tag{34}$$

with periodic boundary conditions in both x and y directions, $f = (16\pi^2 - 1)e^{-t}(\sin(4\pi x) + \sin(4\pi y))$ and properly selected initial condition so that the exact solution is given by

$$u(x, y, t) = e^{-t}(\sin(4\pi x) + \sin(4\pi y)). \tag{35}$$

This problem was solved by the ADI method (10),(11) using the sixth-order scheme (2) to approximate those derivatives. The theoretical accuracy $O((\Delta t)^2, (\Delta x)^6, (\Delta y)^6)$ was confirmed by solving the problem with various mesh sizes and time step sizes. The results presented in Table 3 (with a fixed mesh size) show the convergence rate of $O((\Delta t)^2)$ very well. The results presented in Table 4 (with a fixed small time step) demonstrate the convergence rate of $O((\Delta x)^6)$ very well.

EXAMPLE 3. Consider the Burgers' equation

$$u_t = \nu(u_{xx} + u_{yy}) - (uu_x + uu_y), \qquad (x, y) \in \Omega, \quad 0 < t < 1.25, \tag{36}$$

with appropriate initial and Dirichlet boundary conditions such that the exact solution is given by

$$u(x, y, t) = 1/(1 + \exp(x + y - t)/(2\nu)), \qquad \nu = 0.05. \tag{37}$$

For this nonlinear problem, we solved it by the following ADI method

$$\frac{u_{ij}^{n+1/2} - u_{ij}^n}{0.5\Delta t} = \nu\left[(u_{xx})_{ij}^{n+1/2} + (u_{yy})_{ij}^n\right] - \frac{1}{2}\left[\left(\left(u^2\right)_x\right)_{ij}^n + \left(\left(u^2\right)_y\right)_{ij}^n\right], \tag{38}$$

$$\frac{u_{ij}^{n+1} - u_{ij}^{n+1/2}}{0.5\Delta t} = \nu\left[(u_{xx})_{ij}^{n+1/2} + (u_{yy})_{ij}^{n+1}\right] - \frac{1}{2}\left[\left(\left(u^2\right)_x\right)_{ij}^n + \left(\left(u^2\right)_y\right)_{ij}^n\right], \tag{39}$$

Table 3. Maximum error for Example 2 at $t = 1$ with fixed mesh size $\Delta x = \Delta y = 1/50$.

Time step size	Maximum error	Convergence rate in term of Δt	CPU time in seconds
$\Delta t = 1/10$	7.2469e − 4		4.90 s
$\Delta t = 1/20$	3.1364e − 4	1.2083	9.45 s
$\Delta t = 1/40$	5.7551e − 5	2.4462	17.40 s
$\Delta t = 1/80$	1.4346e − 5	2.0042	33.95 s
$\Delta t = 1/160$	3.5438e − 6	2.0173	67.05 s
$\Delta t = 1/320$	8.4330e − 7	2.0712	133.80 s

Table 4. Maximum error for Example 2 at $t = 1$ with fixed time step size $\Delta t = 10^{-4}$.

Mesh size	Maximum error	Convergence rate in term of Δx	CPU time in seconds
$\Delta x = \Delta y = 1/10$	9.2351e − 4		218.90 s
$\Delta x = \Delta y = 1/20$	1.3497e − 5	5.9470	746.02 s
$\Delta x = \Delta y = 1/40$	2.1695e − 7	5.9591	2695.10 s

where those first and second derivatives and boundary nodes are approximated by those sixth-order formulas presented in Section 2.1. This problem was solved with various time step and mesh sizes. With $\Delta x = \Delta y = 1/20$, $\Delta t = 1/100$, the maximum error is 0.0197, the CPU time is about 11.86 seconds; with $\Delta x = \Delta y = 1/20$, $\Delta t = 1/1000$, the maximum error is 0.0019, the CPU time is about 111 seconds; while using $\Delta x = \Delta y = 1/20$, $\Delta t = 1/10000$, the maximum error is improved to 1.8962e − 4, the CPU time is about 1130 seconds. Here we only observed $O(\Delta t)$ convergence and the error is dominated by the time error. Our explanation for this phenomenon is due to the nonlinear terms, which are approximated at time level n, instead of at time level $n + 1/2$ for the original ADI method for linear problem (see (10),(11)). Figure 1 presents the numerical solutions and pointwise errors at $t = 0.625, 1.25$ obtained with $\Delta x = \Delta y = 1/20$, $\Delta t = 1/10000$. Obviously the numerical solutions are free of oscillation and much better than the results we obtained using RBF meshless method [29], in which case the maximum error is 0.07. We shall further improve the accuracy in time using the computational procedure proposed by Fairweather and Mitchell [30] for ADI methods in the future. Currently we resolved the problem using the classical explicit fourth-order four-stage Runge-Kutta method (RK4), and we found that much more accurate results can be obtained by RK4. For example, with $\Delta x = \Delta y = 1/20$, $\Delta t = 1/100$, RK4 gives the maximum error 2.2562e − 5; and with $\Delta x = \Delta y = 1/40$, $\Delta t = 1/500$, RK4 gives the maximum error 9.4963e − 8, which case is presented in Figure 2.

EXAMPLE 4. We consider a system of nonlinear reaction-diffusion equations [18, p. 351]

$$u_t = u_{xx} + u_{yy} + u^2(1 - v^2) + f(x, y, t), \tag{40}$$

$$v_t = v_{xx} + v_{yy} + v^2(1 - u^2) + g(x, y, t), \tag{41}$$

where f, g, the Dirichlet boundary and initial conditions are chosen accordingly such that the exact solutions are given by

$$u(x, y, t) = e^{-t} \sin(x) \sin(y), \qquad v(x, y, t) = e^{-2t} \sin(2x) \sin(2y). \tag{42}$$

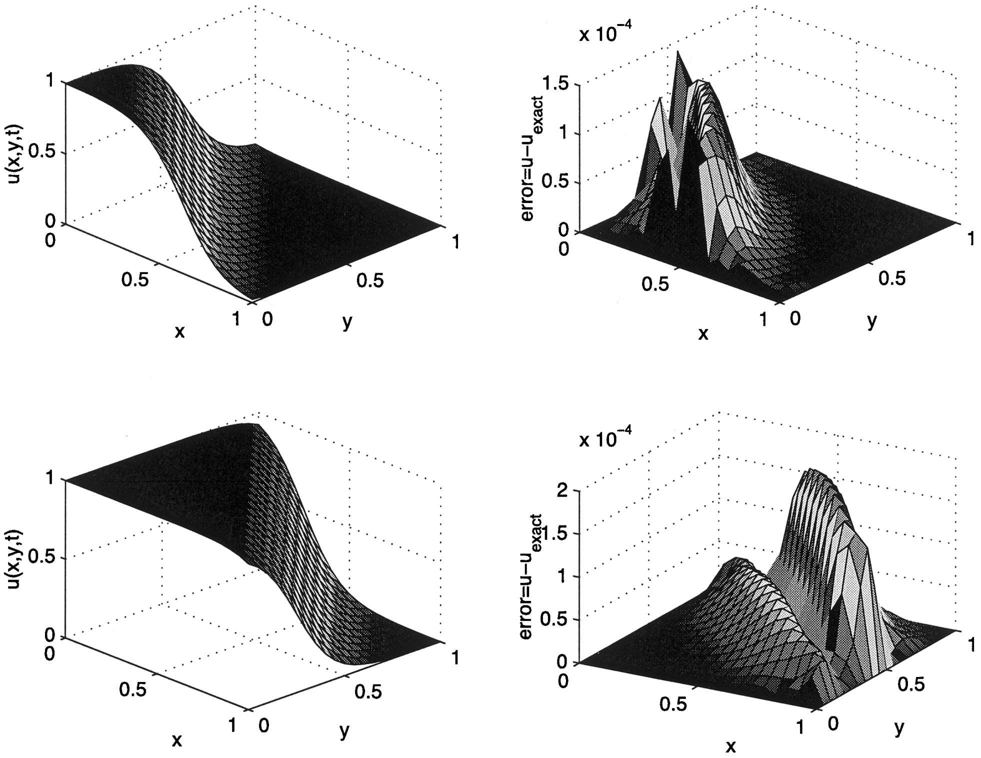

Figure 1. Example 3 (solved by ADI): The numerical solutions (left columns) and pointwise errors (right columns) at $t = 0.625$ (top row) and $t = 1.25$ (bottom row).

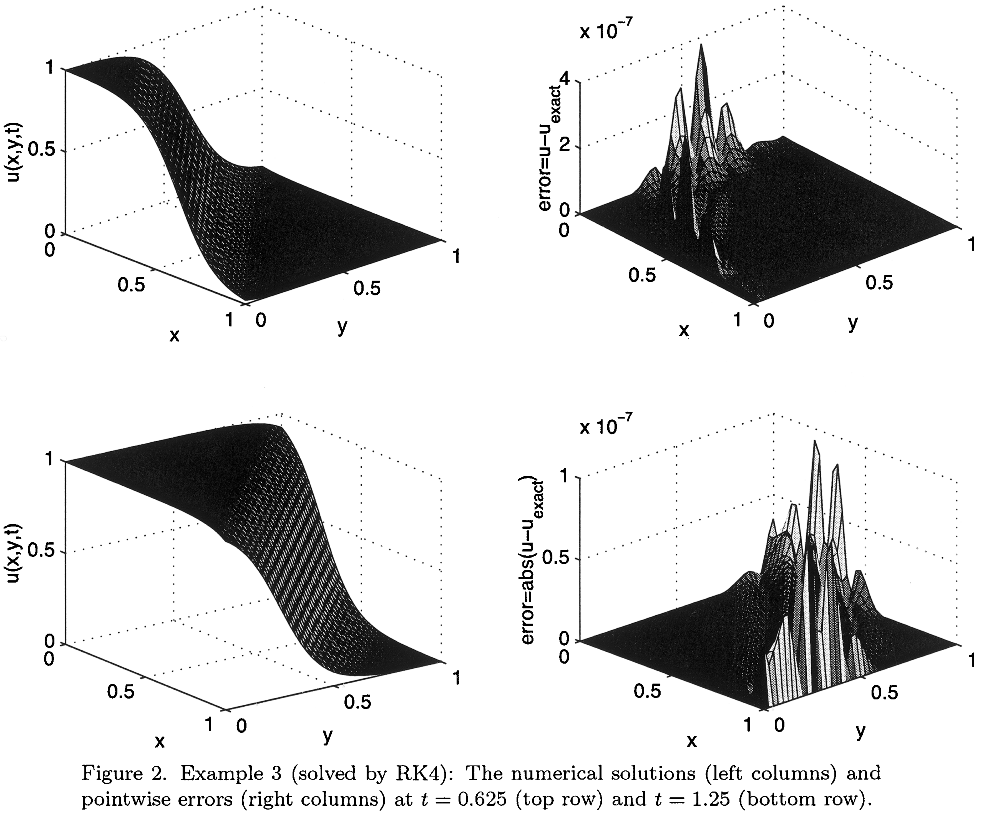

Figure 2. Example 3 (solved by RK4): The numerical solutions (left columns) and pointwise errors (right columns) at $t = 0.625$ (top row) and $t = 1.25$ (bottom row).

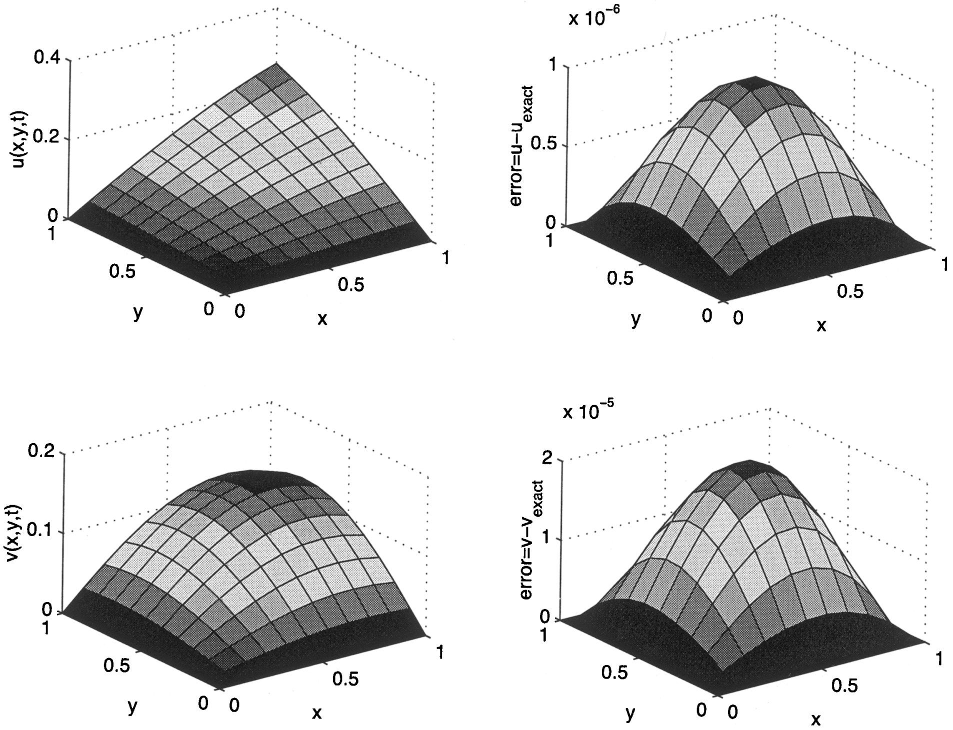

Figure 3. Example 4: The numerical solutions and pointwise errors at $t = 1$. Top row is for u and bottom row is for v.

We solved this problem by the following ADI method

$$\frac{u_{ij}^{n+1/2} - u_{ij}^{n}}{0.5\Delta t} = (u_{xx})_{ij}^{n+1/2} + (u_{yy})_{ij}^{n} + (u^2)_{ij}^{n}(1 - (v^2)_{ij}^{n}) + f(x_i, y_j, t_n), \tag{43}$$

$$\frac{u_{ij}^{n+1} - u_{ij}^{n+1/2}}{0.5\Delta t} = (u_{xx})_{ij}^{n+1/2} + (u_{yy})_{ij}^{n+1} + (u^2)_{ij}^{n}(1 - (v^2)_{ij}^{n}) + f(x_i, y_j, t_n), \tag{44}$$

where those derivatives and boundary nodes are all approximated by those sixth-order formulas presented in Section 2.1. For the equation of v, the scheme is similar.

This problem was solved using different time step and mesh sizes over the time interval $0 \le t \le 1$. We found that the maximum error is dominated by the time error, and the convergence rate in terms of time is $O(\Delta t)$. For example, with $\Delta x = \Delta y = 1/10, \Delta t = 1/1000$, the maximum errors obtained for u and v are $1.8654\text{e} - 6$ and $3.9801\text{e} - 5$, respectively, and the CPU time is 80.20 seconds; while with $\Delta x = \Delta y = 1/10$, $\Delta t = 1/2000$, the maximum errors for u and v are $9.3295\text{e} - 7$ and $1.9905\text{e} - 5$, respectively, and the CPU time is 161.43 seconds. The numerical solutions of u, v and the corresponding pointwise errors obtained with $\Delta x = \Delta y = 1/10$, $\Delta t = 1/2000$ are plotted in Figure 3, which shows that the very accurate solutions can still be obtained by using such a coarse mesh.

5. CONCLUSIONS

In this paper, we develop a sixth-order compact scheme coupled with Alternating Direction Implicit (ADI) methods and apply it to parabolic equations in both 2-D and 3-D. Unconditional stability is proved for linear diffusion problems with periodic boundary conditions. Numerical examples supporting our theoretical analysis are provided. We also implemented our algorithms to nonlinear problems. However, theoretical analysis for the nonlinear problems needs further investigation.

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